315. **ELECTRONIC AND MICROELECTROMECHANICAL SYSTEMS (MEMS) COMPONENTS**
$1,416,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: W. R. Reynolds, (505) 844-3087

This project provides funds to: (1) develop stronglinks in several steps starting with use of micromachining technology to develop parts, then integrate parts to make stonglink; (2) develop all-quartz and integrated silicon-quartz resonators for small clocks and sensors for DOE, military and commercial applications; and (3) develop and characterize low temperature weaklink capacitor and coil and develop/characterize fiber optic sensors.

Keywords: Micromachining, Capacitors, Sensors

INSTRUMENTATION AND FACILITIES

316. **MATERIALS PROCESSES FOR MANUFACTURING**
$703,000
DOE Contact: R. Staffin, (202) 586-7590
SNL Contact: D. L. Lindner (510) 294-3306

This project will consist of two areas to enhance manufacturing capabilities: Virtual Reality and Development Plating Facility. *Virtual Reality* - This project will build on recent developments at Sandia. Free-form rapid prototyping, robotics, on-machine inspection coupled with sophisticated solid models and process models are rapidly emerging areas that will be evaluated and improved. *Development Plating Facility* - Finalize design and complete construction of new Development Plating Facility in the Advanced Manufacturing Process Center (AMPL).

Keywords: Prototyping, Models, Plating

LAWRENCE LIVERMORE NATIONAL LABORATORY

317. **ENGINEERED NANOSTRUCTURE LAMINATES**
$1,800,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Troy W. Barbee, Jr., (510) 423-7796

Multilayers are man-made materials in which composition and structure are varied in a controlled manner in one dimension during synthesis. Individual layers are formed using atom by atom processes (physical vapor deposition) and may have thicknesses of from one monolayer (0.2 nm) to hundreds of monolayers (>100 nm). At this time more than 75 of the 92 naturally occurring elements have been incorporated in multilayers in elemental form or as components of alloys or compounds. In this work deposits containing up to 225,000 layers of each of two materials to form up to 500□m thick samples have been synthesized for mechanical property studies of multilayer structures.

These unique man-made materials have demonstrated extremely high mechanical performance as a result of the inherent ability to control both composition and structure at the near atomic level. Also, mechanically active flaws that often limit mechanical performance are controllable so that the full potential of the structural control available with multilayer materials is accessible. Systematic studies of a few multilayer structures have resulted in free-standing foils with strengths approaching those of whiskers, approximately 70 percent of theory. Also, new mechanisms for mechanically strengthening materials are accessible with nanostructure laminates.

Applications now under development include: coatings for aircraft gas turbine engines; EUV, soft X-ray and X-ray optics spectroscopy and imaging; high performance capacitors for energy storage; capacitor structures for industrial applications; high performance tribological coatings; strength materials; integrated circuit interconnects; machine tool coatings; projection x-ray lithography optics.

Keywords: Thin Films, Multilayer Technology

318. **SOL GEL COATINGS**
$335,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: I. M. Thomas, (510) 423-4430 and
J. Britten, (510) 423-7653

We continue to investigate the preparation of multilayer sol-gel high reflection (HR) coatings using colloidal SiO_2 with either HfO_2 or ZrO_2. We have found that the incorporation of an organic polymer binder such as polyvinyl alcohol or polyvinyl pyrolidinone into the high index component has resulted in an increase in the damage threshold and a decrease in the number of layer pairs required for high reflection.

A laboratory size meniscus coater was evaluated and found to produce mirrors of high optical performance and adequate damage threshold. This is now the preferred method of application, and a large machine capable of producing Beamlet and NIF size mirrors is to be delivered in early FY 1994.

Keywords: Sol Gel Coatings, Meniscus Coater, HR Coatings

319. **KDP GROWTH DEVELOPMENT**
$900,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

Potassium dihydrogen phosphate (KDP) and its deuterated analog (DKDP) are important nonlinear crystals used both for frequency conversion as well as for a large Pockels cell. These crystals are very expensive, due in part to the very long times required to grow large boules (2-3 years) and the cost of D_2O for growing DKDP. We are developing alternative growth techniques to dramatically increase the growth rate of these crystals.

We recently adopted a new growth technique with which we are growing both KDP and DKDP at 10 to 20 times the rates achieved with conventional methods. We have grown crystals up to almost 20cm on a side and have shown that crystals grown by this method are of exceptionally high quality. We are now working with crystallizers that are large enough to grow 50x50x50cm^3 crystals. We will continue to grow crystals at the 10-15cm scale in order to determine optimum hydrodynamic and regeneration conditions, and to understand the effects of impurities and stresses in seed crystals on the stability of the growing crystal face.

Keywords: KDP, Nonlinear Crystals, Crystallization

320. **ICF CAPSULE ABLATORS VIA PLASMA POLYMERIZATION**
$500,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Brusasco, (510) 422-3111, R. Cook, (510) 422-3117 and S. Letts, (510) 422-0937

Our group uses plasma polymerization to prepare conformal coatings of organic polymer for use as ICF capsule ablators. These coatings have some unique and stringent requirements, such as a surface roughness of the order of 10 nm or less at a coating thickness of several tens of micrometers and the strength to hold fuel pressures of from 50 to 100 atmospheres. The project supports development of methods to incorporate high Z dopants (e.g., germanium) into the polymer structure. The project also supports basic studies to understand the mechanism of roughness evolution during deposition and methods to enhance rate without seriously affecting roughness. The incorporation of beryllium into the ablator is also a focal point for exploratory research. A coating system with a computer interface aids the optimization of the coating process.

Keywords: Plasma, Polymer, Germanium, Beryllium, Fusion, Roughness

321. **VICARIOUS NUCLEOPHILIC SUBSTITUTION CHEMISTRY**
$400,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

Vicarious nucleophilic substitution chemistry is being used to synthesize energetic materials. New explosive molecules are being synthesized. Alternate routes to existing molecules, such as TATB , have been developed.

Keywords: Examination, Explosive, Energetic, TATB

322. **CHEETAH THERMOCHEMICAL CODE**
$190,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

A thermochemical code for the prediction of detonation performance is being developed. In addition to detonation performance, thermochemical calculations of impetus and specific impulse for propellant applications may also be made.

Keywords: Examination, Explosive, Energetic, TATB

323. **HARD TARGET PENETRATOR EXPLOSIVE**
$900,000*
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: R. L. Simpson, (510) 423-0379

New explosives are being developed for hard target penetrators. The goals include insensitivity to shock loading and significantly higher energy density than that of currently available materials

Keywords: Explosive

324. **INJECTION MOLDABLE EXPLOSIVES**
$220,000*

Precision explosive materials that may be injection molded are being developed for precision applications.

Keywords: Explosive

---

*General energetic materials-related input. This activity is jointly funded (50:50) by DOE DP and the DoD.

MATERIALS PROPERTIES, BEHAVIOR, CHARACTERIZATION OR TESTING

325. **INTERFACES, ADHESION, AND BONDING**
$460,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Wayne E. King, (510) 423-6547

Our experimental effort is producing results that are directly comparable with theoretical calculations. We are investigating planar metal/metal interfaces and metal/ceramic interfaces (in anticipation of improvements in the theory) of well defined misorientations. In order to span the entire range of length scales described above, macroscopic bicrystals a few millimeters thick, with interfacial areas on the order of a square centimeter, will be required. In order to obtain such bicrystals, we plan to employ the diffusion bonding approach. An ultra-high-vacuum diffusion bonding machine has been developed in parallel with this research project.

Keywords: Interfaces, Bonding, Electronic Structure

326. **LASER DAMAGE: MODELING AND CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: M. R. Kozlowski, (510) 424-5637

We have been working to understand the damage mechanism in thin film coatings used on Nova and other ICF lasers, with the ultimate goal of improving the damage threshold in coatings for future laser systems. We have utilized atomic force microscopy (AFM) and focused ion-beam (FIB) cross sectioning to characterize laser damage as well as the laser conditioning process which allows coatings to sustain higher laser fluences. We have shown that pre-existing nodular defects are the initiation points for most laser damage. The laser conditioning process is associated with the gentle ejection of these nodules to produce benign pits.

We have modeled the laser induced electromagnetic fields at "typical" nodular defects in a simple quarter-wave dielectric mirror coating. The model results demonstrated that large field enhancements are produced by these defects, which are composed of the same dielectric material as the coating materials. We are not calculating the thermal-mechanical response of these defects. Work to date has only looked at the normal incidence illumination case. With recent electromagnetics code advancements, we will now be able to model the more interesting non-normal incidence case.

Keywords: Coatings, Atomic Force Microscopy, Laser Damage

327. **KDP CHARACTERIZATION**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

We require very large, high quality crystals of potassium dihydrogen phosphate (KDP) and its deuterated analogue (DKDP) for present and advanced high power lasers in the ICF Program. The performance of these crystals is limited by strain which induces anomalous birefringence and wavefront distortion and by defects which result in laser-induced damage at low laser fluence. The level of internal strain and the laser damage threshold are the most important factors in determining the yield of useable plates from an "as-grown" boule. Our goal has been to identify the defects which are the source of strain and damage in KDP and DKDP, understand how these defects are generated, and how to avoid them during the growth process.

We are using optical scatterometry, spectroscopy, x-ray typography, crystal growth and chemical analysis to determine the distribution of defects in crystals and their relationship to the growth process. We have been able to relate strain to specific defects using these methods and are now investigating, *in situ*, the process of laser damage as well as laser and thermal annealing.

Keywords: KDP, Strain, Crystal

INSTRUMENTATION AND FACILITIES

328. **SCANNING TUNNELING MICROSCOPY (STM) AND ATOMIC FORCE MICROSCOPY (AFM)**
$250,00
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: W. Siekhaus, (510) 422-6884

A small building standing separate from noise-generating machinery and hence having a low natural vibration background is used to house all scanning probe instrumentation. The large stage scanning probe microscope that can perform scanning tunneling as well as contact and non-contact atomic force microscopy on the surface of objects as large as 6" in diameter, a small-stage non-contact AFM and STM, and an ultra-high vacuum

instrument that can perform non contact AFM and STM measurements and STM spectroscopy (STS) have been used for the following studies in FY 95.

- Uranium Hydriding - Understanding the early stages of uranium hydriding is of paramount importance in science based stockpile stewardship. The UHV STM/AFM has been used to determine the initial stages of uranium hydriding by exposing a clean uranium surface to hydrogen and monitoring by AFM the change in surface morphology induced by hydriding. We have in this way identified with nm resolution the sites at which hydriding starts and monitored the growth of hydride at these sites as a function of time.

- Light-emission from Nanoscale Silicon Particles - Nm-scale clusters of Si have been deposited by laser ablation and by evaporation in a noble gas atmosphere onto the basal plane of graphite, and analyzed by STM to determine their size distribution and by optical spectroscopy to study the physical basis for light-emission from Si clusters and from oxidized Si.

- Dissolution Rate of Uranium Oxide - The transport of radioactive material from a long-term storage site into ground water is of concern in designing long-term storage facilities for nuclear waste material. The dissolution of uranium oxide by ground-water is a rate limiting step in this process. This dissolution rate has been determined by AFM on single crystal uranium oxide by monitoring the rate of recession of the UO_2 surface with reference to a gold marker. Moreover, the nm-scale morphology of the dissolution attack has been identified, showing that some crystallographic directions are preferentially attacked.

Keywords: NDE, Chemical Reaction, Uranium Hydriding, Stockpile Stewardship, Uranium Oxide Dissolution, Nuclear Waste Disposal, Etching, Si Light Emission

329. **TREATMENT OF WASTE AND WATER WITH CARBON AEROGEL ELECTRODES**
$425,000
DOE Contact: Douglas Gish, DP 42, (202) 586-1741
LLNL Contact: J. C. Farmer, (510) 423-6574

Carbon aerogel capacitive deionization (CDI) has been developed as a non-polluting, energy-effecient, cost-effective alternative to ion exchange, reverse osmosis, electrodialysis, and evaporation. This process is believed to offer dramatic advantages in terms of both waste minimization and processing cost to DOD and DOE. The benefits of this project include the elimination of secondary wastes associated with the chemical regeneration of ion exchange columns; the avoidance of flow through porous media as required by reverse osmosis (RO); the elimination of expensive and troublesome high-pressure pumps associated with RO; and the reduction of the required energy consumption to process water. This process could help facilitate low-cost desalination of brackish waste water for reclamation. This SERDP project has been recognized with a 1995 R&D100 Award.

Keywords: Capacitive Deionization

330. **TRILAYER JOSEPHSON JUNCTIONS (TECHNOLOGY TRANSFER INITIATIVE)**
$375,000
DOE Contact: W. T. Chernock, (301) 586-7590
LLNL Contact: R. H. Howell, (510) 422-1977

In this TTI Lawrence Livermore National Laboratory is working with Varian Associates to lay the groundwork for the routine, reproducible fabrication of high-temperature superconducting trilayer structures. The project was completed at the end of FY 1995. Project goals were to: (1) identify high temperature superconducting materials, metallic and insulating barrier materials and associated substrate and electrode materials for engineered trilayer structures that can provide Josephson Junction devices with desired characteristics for sensor or electronic circuit use; (2) identify and test potentially useful analysis techniques and to provide data appropriate for the validation and analysis of the input materials, trilayer structures and completed JJ devices; and (3) to integrate the analysis results with the existing Varian data base to optimize the growth and fabrication process to obtain more reproducible devices across each chip and from chip to chip. All milestones were met. The timing of the milestones was revised midway through the CRADA term to allow a longer time to pursue the objectives at no additional cost to either partner.

Varian Associates used their unique capabilities to fabricate high temperature superconducting thin films layered with other non-superconducting materials and to evaluate them for their suitability for fabrication into electronic devices. These films were made in several configurations using a variety of materials in the superconducting films. Films were then ananlyzed by LLNL using a suite of techniques including Rutherford Backscattering Spectroscopy, Secondary Ion Mass Spectroscopy, Electron Microprobe Analysis, Auger Microprobe Analysis, Ion Microprobe Spectroscopy, Scanning Tunneling Microscopy, Atomic Force Microscopy, Scanning Electron Microscopy and High Resolution Transmission Electron Microscopy. These techniques were first evaluated for their utility in providing useful information regarding either general film quality or the details of defects sometimes found after deposition. Some were then chosen for routine use in subsequent analysis.

Varian Associates have refined their fabrication process as a better understanding of the results of the film deposition grew from the analyses performed at LLNL. These activities constituted the program's main deliverables and were performed at the expected level. Varian Associates are now making the highest quality films of high temperature superconducting layered structures available in the world and are the only growers capable of supplying sufficient uniformity across a film to fabricate multiple electronic devices in an array. Additional development at Varian Associates is required to bring these films to their full commercial potential.

Keywords: Superconductors, High Transition Temperature, Josephson Junction, Tri-layers, Heteroepitaxy

331. **LITHIUM CELL DEVELOPMENT**
$200,000
DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

We completed work on the development of a replacement electrolytic cell for the manufacture of lithium metal in support of the DOE Y-12 facility. Our development incorporates the introduction of a bipolar cell methodology where a bipolar electrode is one that is shared by two cells connected in electrical series. In the process developed, lithium is electrodeposited in an aqueous cell at ~30°C and then anodically removed and recovered as pure lithium at a molten lithium cathode. Lithium-depleted amalgam is returned to the aqueous cell after transferring heat counter-current to the incoming lithium-rich stream. The process eliminates high temperature electrolysis of LiCl and multiple unit processes to produce the anhydrous LiCl feedstock at Y-12. Computer control was rendered operational, but not fully employed. System auxiliaries (hot lithium transfer, vapor condensers, various diagnostics) were fabricated and installed but not fully tested. We established process feasibility by operating an integrated system consisting of aqueous cell, molten salt cell, thermal controls and amalgam circulation subsystems. Finally, we showed experimentally, that process energy efficiencies of 70% could be achieved at practical parameters.

Keywords: Lithium, Bipolar, Electrolytic Cell Development

332. **ENVIRONMENTALLY SAFE DISPOSAL OF EXPLOSIVE WASTES: SERDP PROJECT**
$800,000
DOE Contact: Andre Cygleman, (202) 586-8814
LLNL Contact: John R. Kolb, (510) 422-6424

In collaboration with researchers at Los Alamos National Laboratory and the Pantex Plant, we are exploring options to support the Department of Energy and the Department of Defense in their quest to develop environmentally sound techniques for the destruction of residual high explosive remnants after dismantlement and demilitarization occur. We intend to pursue and have demonstrated positively during this year, the capacity to minimize the amount of high explosive materials to be treated as waste and subsequently destroyed. We have chosen to manage the returning, surplus energetic material as an asset to be sold or given away in lieu of destruction. Through minimization of the amount of HE waste, we believe we can reduce, by an order of magnitude, the amount of material for which environmentally sound disposition techniques must be generated. We have focused on molten salt destruction, base hydrolysis and bioremediation as techniques to be investigated this year. We have also supported a study on the desirability of recycling and reusing insensitive high explosives with a minimum of waste generation or cleanup. No downselection among techniques was possible based on the final results of the study as reported. The effort ended in FY95 and combinations of the three techniques may be used for plant design.

Keywords: SERDP, Environmentally Benign High Explosive Waste Destruction

333. **LAMINATED METAL COMPOSITES FOR AEROSPACE APPLICATIONS**
$700,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (510) 422-9633

Laminated metal composites are materials in which two or more metal containing layers are deformation bonded. Previous work at LLNL has shown that these materials can have properties (such as fracture toughness, fatigue, damping capacity and impact behavior) that are superior to properties currently available in lightweight materials.

These materials also offer the possibility to tailor properties to a prescribed application through the choice of component materials, relative volume fraction of the components, interface strength, etc. This project is funded through the Technology Transfer Initiative and is exploring the application of these materials to fan containment systems for commercial jet engines and to airframe structural components.

Keywords: Materials Properties, Behavior, Characterization or Testing

396. **FATIGUE OF METAL MATRIX COMPOSITES**
$500,000
DOE Contact: Warren Chernock, (202) 586-7590
LLNL Contact: Donald Lesuer, (510) 422-9633

This project involves Lawrence Livermore National Laboratory, Oak Ridge National Laboratory and General Motors. The project is studying the mechanisms of high cycle fatigue in squeeze cast metal matrix composites. The life limiting microstructural features are being determined and the processing-structure-property correlations are being established. Models that can predict lifetimes will be developed.

Keywords: Materials Properties, Behavior, Characterization or Testing

334. **NOVEL MATERIALS FOR OPTOELECTRONICS AND PHOTONICS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: Howard W. H. Lee, (510) 423-5877

This program seeks to develop and implement promising new materials for optoelectronics and photonics that will substantially improve device and system performance and enable new and innovative technologies. Representative materials include nanocrystals, organics (conjugated polymers and small molecules), aerogels, and novel nonlinear optical (NLO) materials such as fullerenes. Our studies on the nonlinear optical properties of fullerenes showed their figure of merit to be very competitive with optical fibers for all-optical switching and have demonstrated the first fullerene-based all-optical switch. Thin films of NLO materials such as fullerenes permit an integrated optics approach which greatly minimizes the latency problem inherent with fiber optics. Other thin film NLO materials were also pursued for these applications. We have developed a type of nanocrystalline silicon (fabricated synthetically and from porous silicon) that photoluminesces throughout the visible. This nanocrystalline silicon is particularly easy to fabricate and can potentially serve as an efficient and inexpensive phosphor or as the luminescent center for flat panel displays and other light emitting applications. Nanocrystals of other materials were also studied. We have also fabricated arrays of miniature junction diodes from porous and nanocrystalline silicon that emit in the visible and near infrared. Silicon-based emitters are desirable because they integrate well with standard silicon-based microelectronics. Finally, we are developing doped aerogels and electroluminescent organic materials (conjugated polymers and small molecules) for light emissive applications such as light emitting devices, flat panel and three-dimensional displays.

Keywords: Optoelectronics, Photonics, Nanocrystals, Porous Silicon, Fullerenes, Polymers, Aerogels, Electroluminescence, Flat Panel Displays, All-Optical Switching

335. **NOVEL MATERIALS STUDIES AT HIGH PRESSURES AND TEMPERATURES**
$400,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contact: Choong-Shik Yoo, (510) 422-5848

The objective of this project is to study the direct elementary energetic reactions among particularly the 1st and 2nd row elements and diatomic molecules, by using a diamond-anvil cell laser-heating technique combined with synchrotron x-ray diffraction and micro-Raman spectroscopy. The feasibility of this experimental approach has well been demonstrated in our recent melting and phase transition studies of iron and actinides performed in an extended region of pressure to 1.3 Mb and temperature to 4000 K. In addition, this technique is also applicable to various energetic materials studies, including synthesis of a new class of energetic materials, electronic structures and metalization, hot spot initiation and laser combustion, at high pressures and temperatures.

Because the reactivity of materials increases substantially at high pressures and temperatures, we have been able to study highly energetic, elementary reactions between simple diatomic molecules (nitrogen, oxygen, and hydrogen) and light elements (B, Al, C, Si, etc.) or transition metals (Mg, Fe, U, etc.) at high pressures and temperatures. These reactions yield various technologically important oxides, nitrides, and hydrides, whose crystal structures can be modified by the P,T- conditions. We have also found that many of these reactions proceed extremely exothermically and can be used for metal combustion applications and/or for potential high explosives. For example, the oxidation reaction of uranium at 1 Mb and 2000 K releases extremely high transient energy which increases the temperature high enough to melt diamond (probably above 7000 K). The direct nitration reactions of boron and carbon proceed highly exothermically and yield

novel materials like c-BN and various hard carbon nitrides. These kinds of energetic reactions could be of interest to DoE and DoD.

Keywords: Novel Materials Applications; Energetic Metastable Materials; Nitrides, Hydrides, Oxides and Ceramics; X-ray Laser Heating Experiments; High Pressures and Temperatures

336. **MATERIALS PRODUCED WITH DYNAMIC HIGH PRESSURE**
$400,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: William Nellis, (510) 422-7200

This project produces novel materials (crystal structures, microstructures, and properties) using high shock pressures. The terms dynamic and shock are used synonymously in this context. Tuneable shock pressure pulses are produced by the impact of a projectile launched from a small two-stage light-gas gun. Shock pressures range from 0.01-1 Mbar, temperatures range from 50 up to a few 1000°C, strain rates on loading range above 10^8/s and quench rates on release of pressure are 10^{12} bar/s and 10^9 K/s in specimens which are recovered intact for investigation. A gas gun is used to achieve these high shock pressures. Specimens range from 1 micron to 3 mm thick and from 3 to 23 mm in diameter. The observed material structures are correlated with computational simulations to enhance understanding of the effects produced. For example, a computational model of the dynamic compaction of nanocrystalline Al particles was shown to be in good agreement with the structure of compacts produced experimentally. A wide variety of materials characterization measurements are made both before and after application of high dynamic pressures, including x-ray diffraction, TEM, SEM, magnetization, NMR, and neutron scattering. In the past year we have dynamically compacted nanocrystalline Al, ceramic, and magnetic powders, produced unusual glass in bulk and nanocrystalline Si in grain boundaries by shock compressing quartz single crystals, and investigated impacts in nature by studying structural effects in shocked minerals. This shock method can be used to produce nanocrystalline particles of many materials contained initially in single crystals.

Keywords: Shock Pressures, Gas Gun, Materials Characterization, Ceramics, Magnets, Nanocrystalline Si, Glass

337. **PROPERTIES OF HYDROGEN AT HIGH SHOCK PRESSURES AND TEMPERATURES**
$300,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: William Nellis, (510) 422-7200 and Neil Holmes, (510) 422-7213

The properies of hydrogen at high pressures and temperatures are a "Holy Grail" issue for laser fusion, condensed matter physics, and planetary physics. Hydrogen in the form of deuterium-tritium is the fuel in laser fusion targets; the metallization of hydrogen by electronic bandgap closure has been a key goal of condensed matter physics since the early part of this century: and Jupiter with its 300 Earth masses is 90 percent hydrogen at high pressures and temperatures. This project measures temperatures and electrical conductivities of cryogenic liquid hydrogen and deuterium shock-compressed to pressures up to 2 Mbar ($2x10^6$ bar) and temperatures up to 5000 K with a two-stage light-gas gun. These conditions are achieved by impact of projectiles accelerated to velocities up to 8 km/s. Shock temperatures up to 5000 K at 1 Mbar were measured by a fast optical spectrometer and show that hydrogen undergoes a continuous dissociative phase transition above 200 kbar. This continuous dissociation absorbs energy, which causes lower temperatures and higher densities in the Mbar shock pressure range than was thought previously.

Electrical conductivities were measured using metal electrodes at pressures in the range 1 to 2 Mbar at calculated temperatures of 2000 to 4000 K. A novel technique was used to produce just enough shock heating to excite just enough electronic carriers to be able to measure the electrical conductivity of hydrogen at Mbar pressures in the short time duration of the experiment. Ours are the only electrical conductivity measurements on condensed hydrogen at any pressure. We have, for the first time, metallized hydrogen at 1.4 Mbar and 3000 K in the fluid and determined the density dependence of the electronic bandgap in the molecular fluid phase. Our observed metallization pressure in the fluid is about one-half what was predicted for the solid at 0 K. Both molecular dissociation and electronic excitation (ionization) affect the hydrogen equation of state to make hydrogen more compressible than believed previously and, thus, facilitate laser fusion. We are the first to metallize hydrogen. Our improved hydrogen equation of state has produced an improved picture of the interior structure of Jupiter and we can now determine the electrical conductivity of hydrogen

throughout the interior of Jupiter. The electrical conductivity determines the large magnetic field, which is about fifteen times larger than the Earth's.

Keywords: Shock Pressures, Shock Temperatures, Electrical Conductivities, Gas Gun, Hydrogen, Cryogenics, Equation of State, Dissociation, Metallization

338. **LOW DENSITY FOAM SHELLS FOR CRYOGENIC ICF EXPERIMENTS**
$600,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contacts: R. Cook, (510) 422-3117

This program has as its goal the development of foam shells, from 1 to 2 mm in diameter with 100 μm foam walls whose density is 50 to 75 mg/cc and whose cell size is less than 1 μm. These shells must also have a 5 to 10 μm thick full density overcoat, and the outer surface finish must be better than 0.1 μm. Foam and overcoat must be composed of atoms with Z less than 9. These foam shells will be used to enhance the surface smoothness of solid DT layers in ICF experiments. The shells are formed using microencapsulation techniques. The foam material is based on a resorcinol-formaldehyde (R/F) foam chemistry. Optically transparant shells with 2 mm diameters and 100 μm thick walls have been prepared.

Keywords: Polymers, Laser Fusion Targets, Low Density Foam

339. **ATOMIC LEVEL EXPLOSIVE CALCULATIONS**
$400,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Larry Fried, (510) 422-7796

A package of atomic-level calculations has been assembled that will allow design of new explosive molecules. The package includes calculations of solid density, heat of formation, chemical stability and sensitivity. This package is being tried on various new postulated compositions in concert with feedback from three organic and inorganic synthesis chemists. The intent is to couple Molecular Design with actual synthesis routes at the start so that the final selected design will be something with a good chance of being made in the lab. The target is to provide 10 to 15 percent more detonation energy than CL-20 with no decrease in sensitivity.

Keywords: Energetic Materials, High Explosives, Molecular Design, Detonation

340. **EXPLOSIVE EQUATION OF STATE**
$700,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Clark Souers, (510)-423-4217

Detonation Equation of State research is proceeding on a broad front. Reaction zones and detonation front curvatures have been correlated and a certain capacity for prediction created. The Bigplate design provides an Equation of State with a continuous set of angles of incidence on copper that vary from 0° to about 70°. A JWL system method has been constructed that allows direct comparison between different explosives. It also provides a method for recalculating JWL's at slightly different densities. The failure of the JWL system indicates that the measurement is inside the reaction zone of the explosive. On-going efforts continue to seek a simple way to use Ignition & Growth for prompt detonation.

Keywords: Energetic Materials, High Explosives, Detonation, Equation of State

341. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$236,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: Andrew McMahan, (510) 422-7198 and Albert Holt, (510) 423-4126

Ab-initio theoretical methods are being used to predict and characterize novel high energy density materials. The class of metastable solid phases being explored is characterized by extended and continuous networks of covalent or metallic bonds, without the weak van der Waals links of familiar chemical fuels, propellants, and explosives. One of the most promising candidates investigated previously in this project is a phosphorus-like or polymeric form of nitrogen which should have a stored specific energy per unit volume about three times that of the HMX explosive. More recent work has considered boron hydrides, and in particular suggests that a boron equivalent of the observed aluminum trihydride should be metastable at atmospheric pressure with a hydrogen storage capacity per volume about two and a half times larger than cryogenic liquid hydrogen. All of these new phases are predicted to be high pressure stable, suggesting a natural synthesis route, which is being explored at LLNL by H. E. Lorenzana and collaborators.

Keywords: Energetic Materials, High Energy Density Materials, Atomic-level Materials Modeling, *Ab-initio* Electronic Structure Methods

342. **METASTABLE SOLID-PHASE HIGH ENERGY DENSITY MATERIALS**
$535,000
DOE Contact: Maurice Katz, (202) 586-5799
LLNL Contacts: H. Lorenzana, (510) 422-8982 and M. Finger, (510) 422-6370

Current conventional energetic compounds rely on strong covalent bonds within individual molecules for energy storage. These molecular liquids or solids are characterized by *large equilibrium volumes* resulting from weak van der Waals interactions between neighboring molecules. Our goal is to demonstrate proof-of-principle synthesis of new compounds that achieve an unprecedented enhancement in energy density by completely replacing these weak van der Waals interactions with highly energetic covalent bonds. Recent theoretical studies at LLNL and elsewhere indicate that solid-state phases having uniform and continuously bonded networks (extended solids) offer entirely new and unexplored opportunities as novel energetic materials. These novel systems represent the analog of infinite, energetic molecules. Specifically, a parallel theory effort at LLNL has predicted that nitrogen can be stabilized under ambient conditions in a three-dimensional, continuously bonded configuration characterized by a stored energy per unit volume of 34 KJ/cm^3, about *three times* that of typical monofuels such as hydrazine as well as fuel mixtures such as gasoline/liquid O_2. The recent adaptation of laser heating methods to the diamond-anvil-cell (DAC) offers the most promising synthesis route for proof-of-existence demonstration of these novel high-pressure phases, given the technique's diagnostic versatility and controlled access to extremes of pressure and temperature. Our preliminary experimental results at high pressures indicate substantial weakening of the N_2 triple bond, a necessary condition to synthesizing the polymeric nitrogen phase. On another front, we have begun studies on carbon monoxide, a compound that is isoelectronic with nitrogen and exhibits very similar high pressure phase transformations. Carbon monoxide polymerizes under pressure into a solid that can be recovered and may be energetic. The class of materials proposed here represent a radically different approach to energy storage that remains unexplored.

Keywords: Energetic Materials, High Energy Density Materials

343. **AFM INVESTIGATIONS OF CRYSTAL GROWTH**
$210,000
DOE Contact: G. J. D'Alessio, (301) 903-6688
LLNL Contact: J. J. DeYoreo, (510) 423-4240

The nanometer-scale morphology of crystalline surfaces exerts a strong control on materials properties and performance. While many researchers have studied vapor deposited metal and semiconductor surfaces grown far from equilibrium, few studies have given attention to the morphology of crystal surfaces grown from melts or solutions near equilibrium despite the fact that most bulk crystals are grown in this regime. Understanding the mechanisms of growth and the origin of defects in such crystals can impact materials performance in a number of fields including optics, electronics, molecular biology, and structural biology. We are using atomic force microscopy (AFM) to investigate the growth of single crystal surfaces from solution in order to determine the mechanism of growth, the kinetics of step advancement, the effect of impurities, and the origin of defects.

In 1995 we performed both *ex situ* and *in situ* AFM measurements on three systems, the ionic crystal KH_2PO_4 (KDP), the canonical solution grown crystal, and the protein crystal Canavalin, a prototypical macromolecular biological crystal and crystals of the Sattelite Tobacco Mosaic Virus (STMV). Our results have provided insight into the mechanisms of growth step kinetics and defect incorporation in these systems. In 1996 we will investigate the effect of impurities on step dynamics in these systems and begin to explore the process of biomineralization.

Keywords: Morphology, Crystal Surfaces, Atomic Force Microscopy

344. **SUPERPLASTIC FORMING OF STAINLESS STEEL AUTOMOTIVE COMPONENTS**
$150,000
DOE Contact: M. Michaelis, (202) 586-4105
LLNL Contact: J. W. Elmer, (510) 422-6543

Superplastic forming of automotive exhaust components is being investigated as a possible method for fabrication of low emission exhaust systems. Development of a superplastic stainless steels alloy that will meet the required fabrication and performance criteria is being performed. This alloy must be laser welded and superplastically formed to yield a component that maintains a high resistance to exhaust gas degradation during operation. To date welding and superplastic forming of a baseline stainless steel alloy has been demonstrated. New work will focus on continued development of superplastic stainless steel alloys, and testing of laser welded and superplastically formed exhaust system segments.

Keywords: Superplastic Forming, Stainless Steel Alloys, Laser Welding

345. **FORMABILITY AND JOINING ANALYSIS FOR SUPERPLASTIC PANEL DESIGN**
$360,000
DOE Contact: J. Van Fleet, (202) 586-5782
LLNL Contact: J. W. Elmer, (510) 422-6543 and D. J. Trummer, (510) 423-8848

The fabrication of internally stiffened aerospace panel components is being investigated. These panels are fabricated by welding and superplastic forming. Numerical modeling of the forming behavior of titanium and aluminum alloy panels is being performed to predict superplastic pressure schedules and to optimize weld placement. The numerical models developed here will be used as a design tool to help reduce the cost and lead time required to fabricate these panels by conventional trial and error methods.

Keywords: Superplastic Forming, Numerical Modeling, NIKE-3D, Laser Welding, Titanium Alloys, Aluminum Alloys

346. **MICROSTRUCTURAL EVOLUTION IN WELDS**
$330,000
DOE Contact: Bharat Agrawal, (301) 903-2057
LLNL Contact: J. W. Elmer, (510) 422-6543 and Joe Wong, (510) 423-6385

Although welding is an established technology used in many industrial settings, it is least understood in terms of the phases that actually exist, the variation of their spatial disposition with time, and the rate of transformation from one phase to another at various thermal coordinates in the vicinity of the weld. With the availability of high flux and, more recently, high brightness synchrotron x-radiation sources, this work develops *spatially resolved x-ray diffraction (SRXRD)* for in-situ investigations of phase transformations in the heat affected zone (HAZ) of fusion welds. In this investigation, SRXRD will be used as a direct method for monitoring the phases present during welding of titanium in order to track the time-temperature history of welding-induced phase transformations. Results of these experiments will be used to aid in the numerical modeling of the kinetics of phase transformations under the highly non-isothermal conditions that exist in the HAZ of welds.

Keywords: Synchrotron Radiation, X-ray Diffraction, In-Situ Experiments, Phase Mapping, Arc Welding, Titanium, Non-isothermal, Phase Transformation Kinetics

347. **URANIUM CASTING PROGRAM**
$1,000,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

The uranium casting program is addressing the use of permanent molds for near net shape castings, controlled cooling for segregation and microstructure control and the effect of alloy additions and subsequent heat treatment on microstructure. Process modeling has played a key role in producing high quality castings in uranium and uranium alloys.

Keywords: Uranium Casting

348. **URANIUM SPIN FORMING**
$1,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

Spin forming is being explored as a method to produce near net shape wrought uranium components. Process modeling has been useful in predicting stress/strain distribution and spring back. Near net shape components have been produced

Keywords: Spin Forming

349. **PLUTONIUM NEAR NET SHAPE CASTING**
$2,500,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

Near net shape casting is being explored using permanent molds. High quality castings have been produced. Process modeling has played a significant role in defining conditions needed for solidification control.

Keywords: Shape Casting

350. **ELECTRON BEAM COLD HEARTH MELTING OF URANIUM**
$900,000
DOE Contact: Marshall Sluyter, (301) 903-5491
LLNL Contact: Steve Root, (510) 423-5216

An existing electron beam evaporation chamber has been modified to produce controlled solidification uranium alloy ingots. Scrap feeders of various types are being evaluated. High quality ingots which meet the applicable uranium alloy specification have been produced.

Keywords: Electron Beam Melting, Uranium